Priority Programme 1473: „Materials with New Design for Improved Lithium Ion Batteries – WeNDeLIB“

„Thermodynamics and kinetics for stabilization of conversion-type electrodes for LIB based on nano 3d transition metal oxide composites“

Subproject 4 “Influence of electrolyte on stabilization of 3d transition metal oxide composites in conversion type electrodes for LIB”

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The major objective of the research in this sub-project is the deeper understanding of the interphase between cathode material and the electrolyte. Despite extensive studies, even in the most common occurrence of such an interphase (on carbon anode material), the exact reactions and composition of this phase are still subject to scientific disputes. The interface or phase on the cathode side is even more subject to speculation. Due to the fact, that some active materials such as silicon anodes or the conversion type cathodes, as studied here show severe volume expansion of several 100%, the surface of these active materials severely changes during the lithiation and delithiation. An increased understanding of the behaviour of the electrolyte at such surfaces and its capability to form a "flexible" interphase between itself and the active material will greatly improve the controllability of these systems. In order to achieve such goals, initially available materials will be combined to design an electrolyte with desirable properties such as: Ionic conductivity, ion pair dissolution/solubility, electrical stability, chemical stability, thermal stability, low corrosion against aluminum, and passivation and protection of the active material by formation of an SEI. In order to achieve this goal, the impact of the three major components of solvent based electrolyte systems (solvent, Li-salt, additives) will be systematically investigates through electrochemical and spectroscopic analysis. Besides $LiPF_6$, $LiBF_4$ and other frequently used salts further promising candidates like LiBOB (Lithium Bisoxalatro Borat) in organic solvents will be studied. Also small amounts of additives have shown to have severe and selective impact on the formation of SEIs as well as the stabilization of the cathode material. Since limited knowledge has been gathered here despite significant scientific interest, this will be a key field of interest during this study.

We utilize a wide range of electrochemical characterization methods supported by additional *in-situ* and *post mortem* analysis of the investigated cells and materials. The typical set of electrochemical characterization will contain cell testing of half and full cells (c-rate dependent capacity and reversibility), conductivity measurements, determination of the electrochemical stability window of the electrolyte, corrosion of active material by the electrolyte, lithium plating/stripping, electrochemical impedance spectroscopy and the characterization of decomposition products by various analytical methods like GC-MS and ionchromatography. In order to further investigate the SEI formation and the stability of the cathode material, photoelectron spectroscopy (XPS), FTIR analysis, Raman spectroscopy and X-ray powder diffraction (XRD) will be applied.